

Atomistically-informed Mesoscale Simulation of Polycrystalline Materials

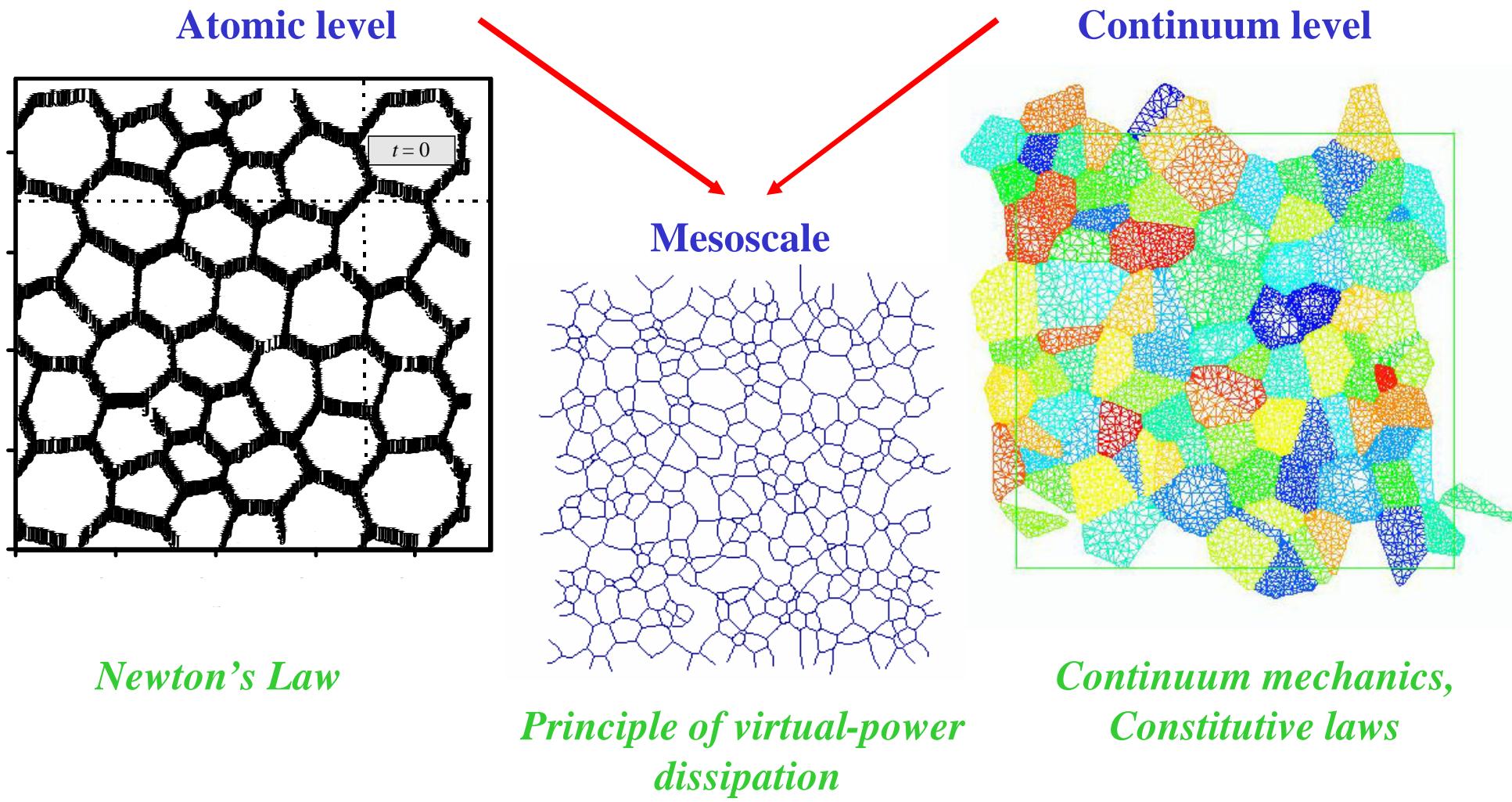
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(after April 1 at Idaho National Lab.)



Scientific Opportunity: Hierarchical Multi-scale Simulation of Polycrystalline Materials



- ‘*Microstructure and deformation physics*’ of nanostructured materials by MD!
- *Continuum simulations based on fundamental understanding of GB physics!*



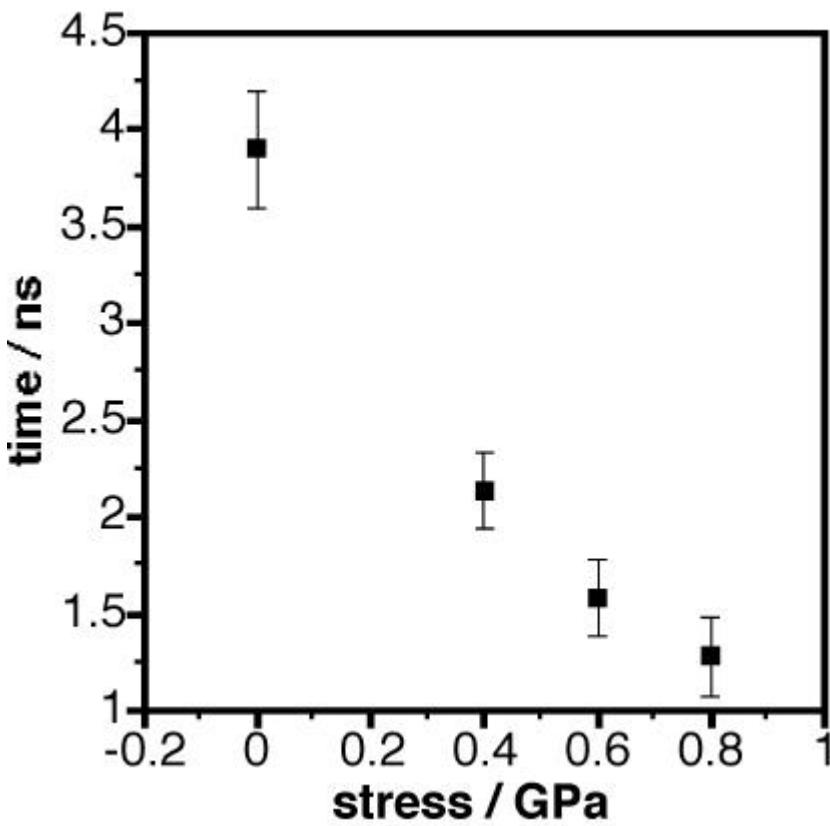
$S = 0.6 \text{ GPa}$
 $T = 1200\text{K}$
($T_m \sim 1500 \text{ K}$)

QuickTime™ and a GIF decompressor are needed to see this picture.

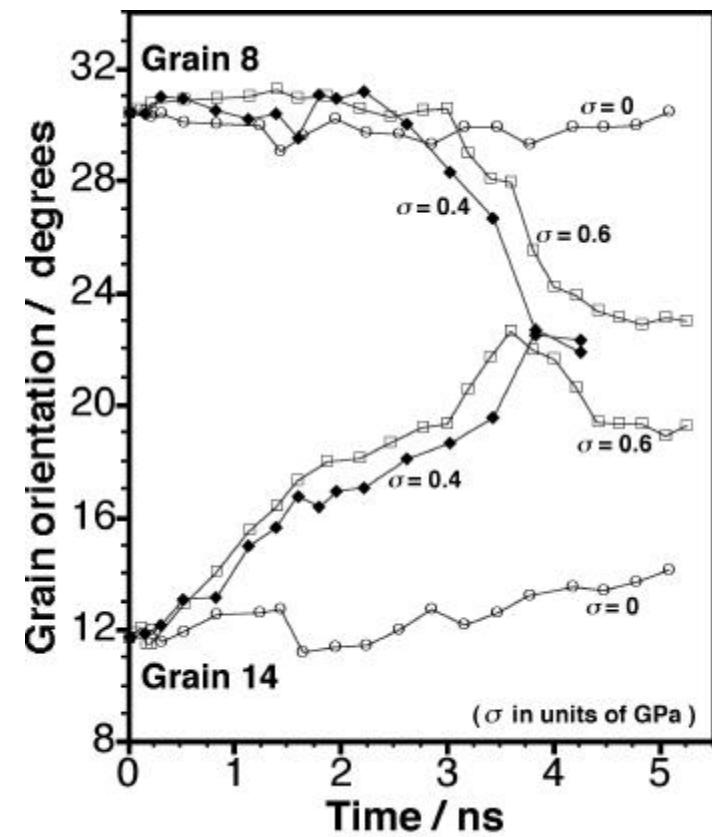
How does stress affect the grain growth?

(A. Haslam et al., *Acta mater.* 51, 2097, 2003)

Time to the disappearance of grain 23
by GB migration



Coupled rotations of grains 8 and 14

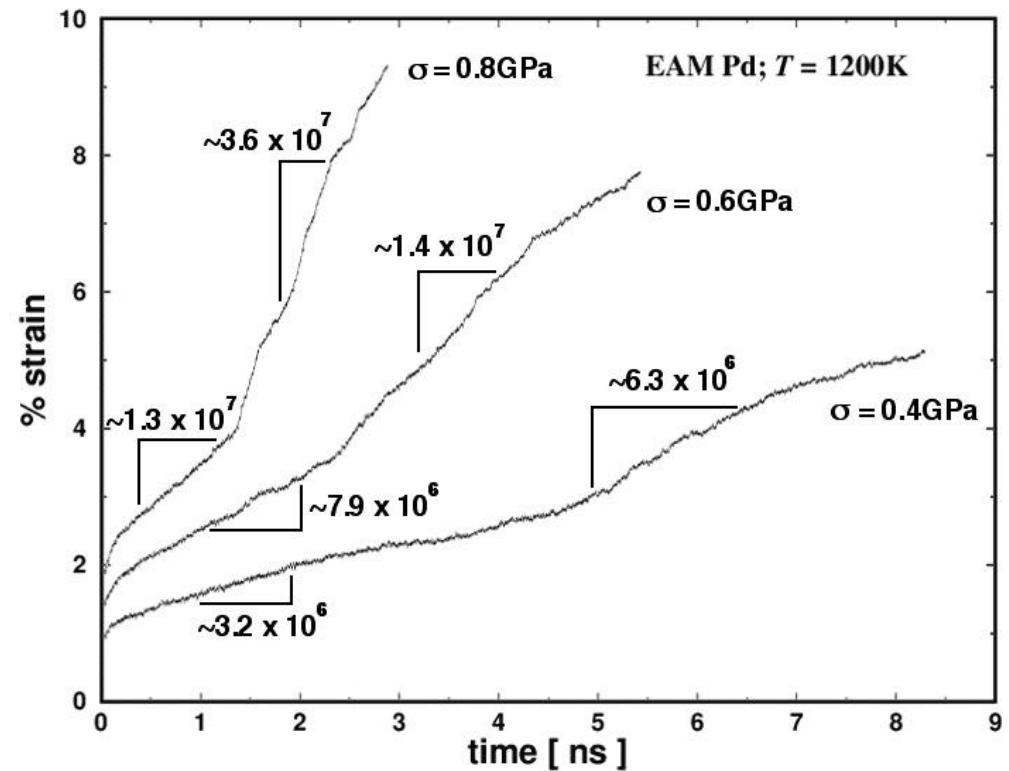
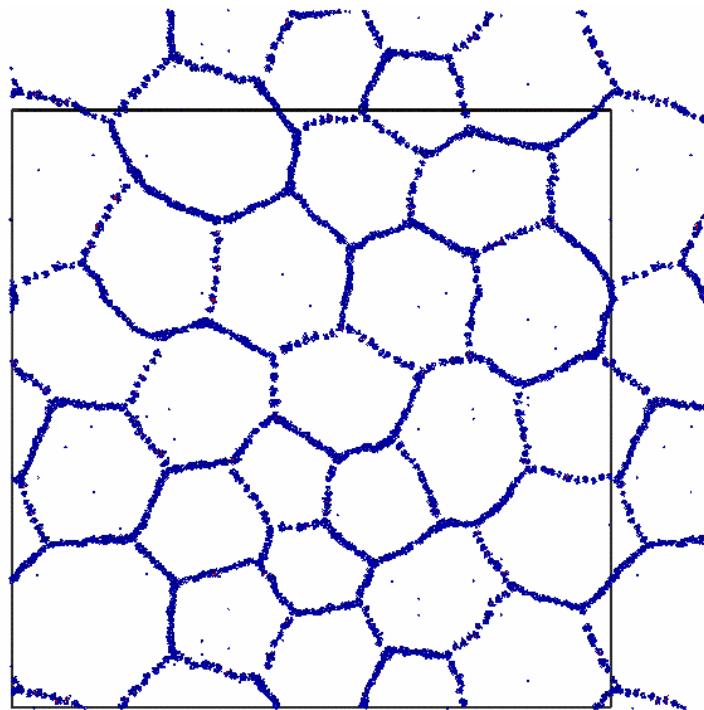


Stress speeds up GB migration!

Stress speeds up grain rotations!

How does grain growth affect the creep deformation?

(A. Haslam et al., *Acta mater.* 52, 1971, 2004)

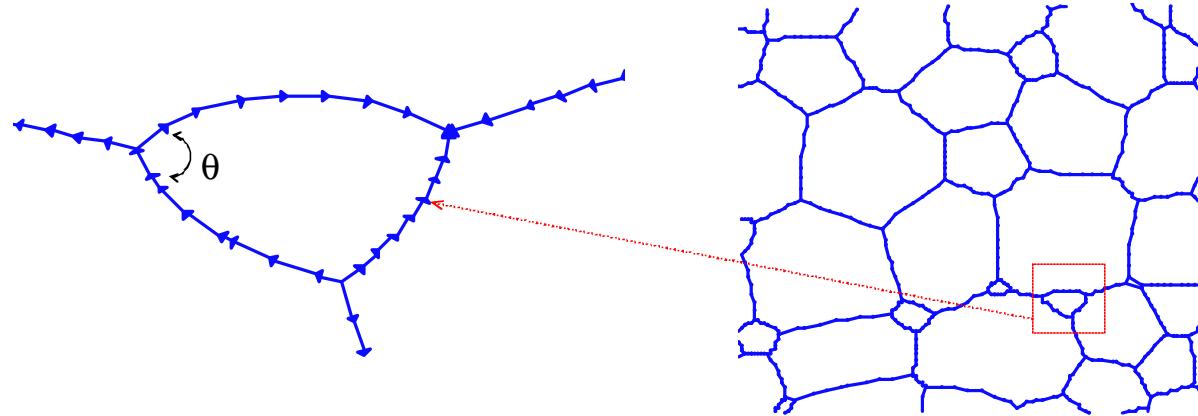


Onset of grain growth speeds up the creep deformation!

Mesoscale Simulations (2d)

(D. Moldovan et. al., Phil. Mag. A 82, 1271, 2002)

- Discretized GBs:



- Variational functional for dissipated power (Cocks 1992, Needleman & Rice 1980, see also Ziegler, *Introduction to Thermomechanics*, 1977):

$$\Pi_m(v; k, \gamma, \mu) \quad \Pi_r(\omega; \tau, M)$$

GB velocity Local GB curvature GB energy GB mobility Angular velocity Torque Rotational mobility

- Viscous force laws: *Replaces Newton's law! Terms are additive!*

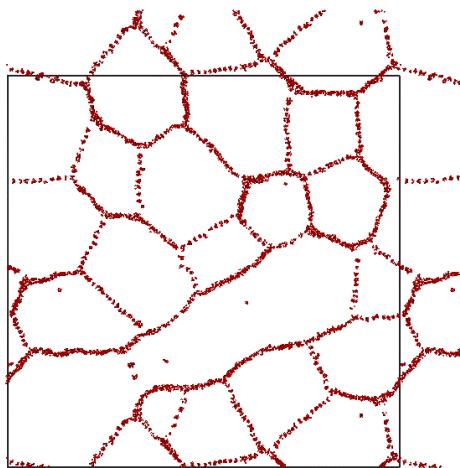
$$v = mg/r; \quad w_i = M_i t_i; \quad M_i \sim d^{-5}; \quad w_i \sim d^{-4}; \quad (\text{D. Moldovan et al., Acta mater. 49, 3521 2001})$$

- Velocity Monte-Carlo or FEM Simulation (F. Cleri, *Physica* 282, 339, 2000; Cocks, 1992)
- Triple-point equilibrium condition (Herring relation) not enforced *a priori*.

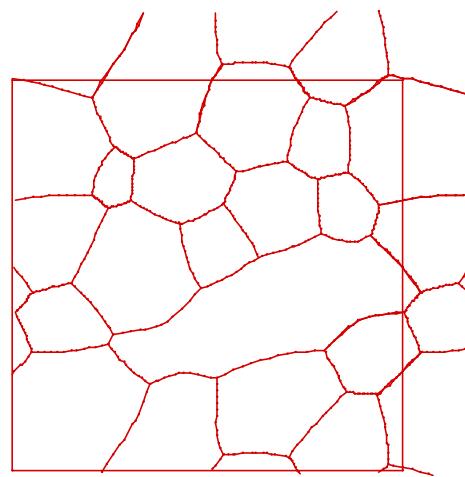
Validation of mesoscale approach against MD simulations

(D. Moldovan et al., Phil. Mag. 83, 3643, 2003)

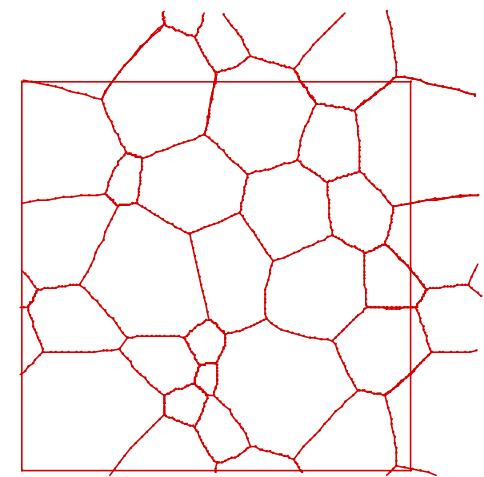
MD: t = 2.89 ns



meso **with** grain
rotation: t = 2.47 ns



meso **without** grain
rotation: t = 2.64 ns



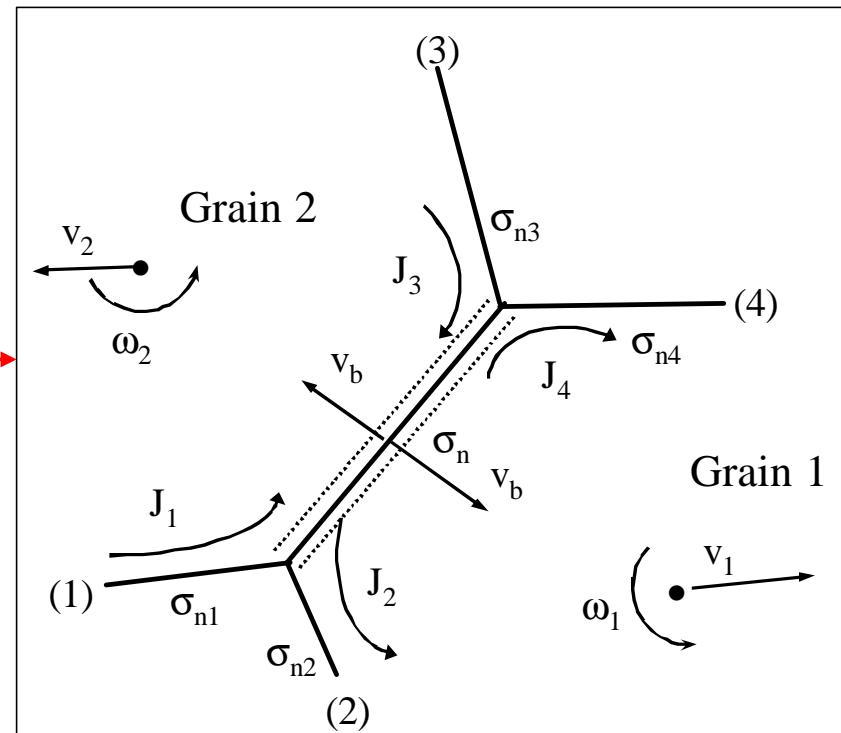
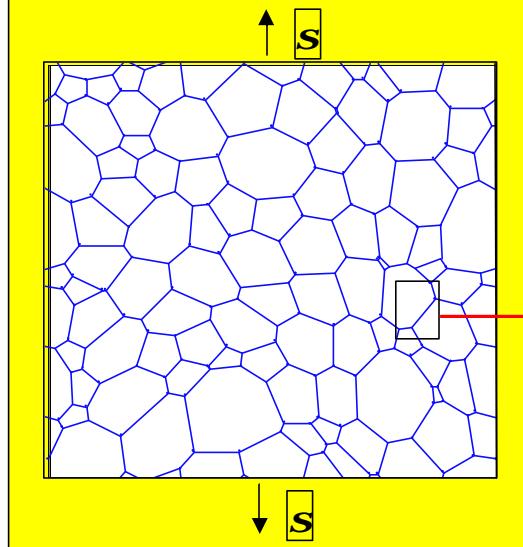
Newton's laws for atoms

*Dissipative dynamics for GBs based on virtual
power dissipation*

- *Distinct processes enter as additive terms in the power functional: dislocations, GBs,...*
- *Ability to deconvolute interplay between distinct processes and driving forces!*

Mesoscale approach to the Coble-creep problem

(A.C.F. Cocks and A.A. Searle, Mech. Mater. 12, 279, 1991)



$$\mu = \mu_0 - \sigma_n \Omega$$

$$J = \frac{D_b \delta_b \Omega}{kT} \frac{d\sigma_n}{ds}$$

$$\frac{\partial J}{\partial s} + v_n = 0$$

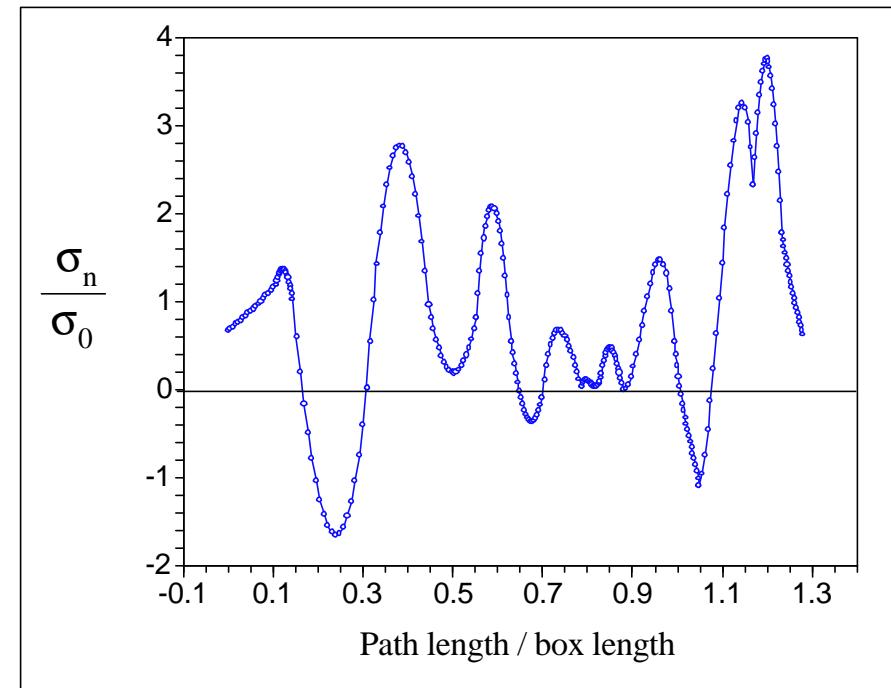
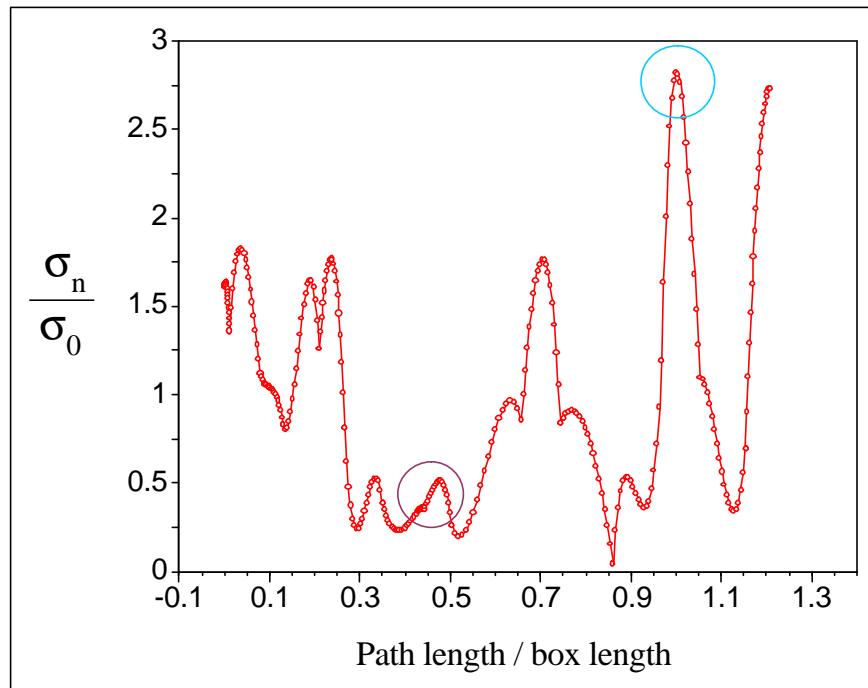
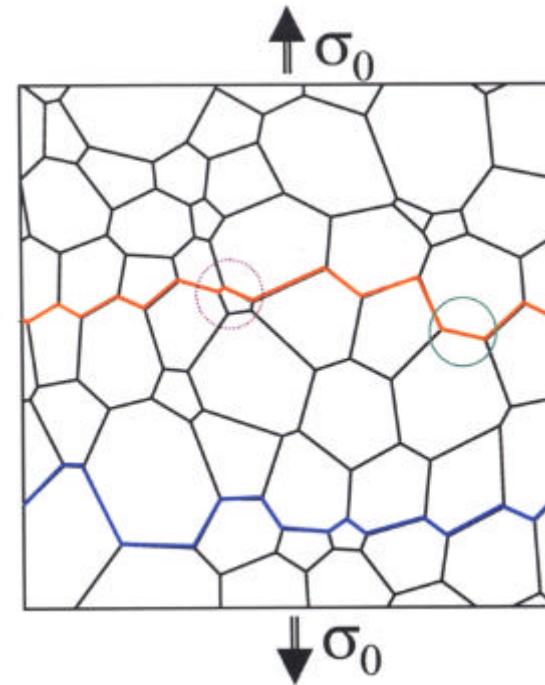
$$\sum_{TJ rays} J_i = 0$$

Variational Functional for a GB segment

$$\Pi_0 = \int_s \frac{kT}{2D_b \delta_b \Omega} J^2 ds - \int_S T_\alpha v_\alpha dS$$

- grains can translate and rotate as rigid units

GB normal stress along two different paths in an irregular 62-grain microstructure:



What is most needed?

- Fully incorporate mesoscale approach into a meshfree approach
 - *Result will be a powerful combined front-tracking & meshfree FEM approach which can be extended to 3d systems*
- Incorporate ion irradiation into mesoscale approach
 - *Interaction of point defects with microstructure (dislocations, grain and phase boundaries)*
- Incorporate microcrack formation and propagation
- Incorporate dislocation-GB processes and dislocation processes in the grain interiors